S-matrix theory of single-channel ballistic transport through coupled quantum dots

I. Rotter[1] and A.F. Sadreev[2,3]

[1] *Max-Planck-Institute für Physik komplexer Systeme, D-01187 Dresden, Germany*

[2] *Kirensky Institute of Physics, 660036, Krasnoyarsk, Russia and*

[3] *Department of Physics and Measurement Technology,*

Linköping University, S-581 83 Linköping, Sweden

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Abstract

We consider single-channel transmission through a double quantum dot system that consists of two single dots coupled by a wire of finite length L. In order to explain the numerically obtained results for a realistic double dot system we explore a simple model. It consists, as the realistic system, of two dots connected by a wire of length L. However, each of the two single dots is characterized by a few energy levels only, and the wire is assumed to have only one level whose energy depends on the length L. The transmission is described by using S matrix theory. The model explains in particular the splitting of the resonant transmission peaks and the origin of the transmission zeros. The latter are independent of the length of the wire. When the transmission zeros of the single dots are of first order and both single dots are identical, those of the double dot are of second order. First-order transmission zeros cause phase jumps of the transmission amplitude by π, while there are no phase jumps related to second-order transmission zeros. In this latter case, a phase jump appears due to a resonance state whose decay width vanishes when crossing the energy of the transmission zero.

I. INTRODUCTION

Advances in nanotechnology have made it possible to fabricate quantum dots (QDs) and to study their transport properties. Single quantum dots can be considered as artificial atoms if the energy levels can be resolved. Two or more QDs can be coupled to form an artificial molecule, in which the electrons are shared by different sites. Recently, much interest is devoted to the study of the properties of these coupled QDs or artificial molecules [1]. One of the most important challenges is to understand the basic properties of coupled QDs since they display the simplest structures of quantum-computing devices that can be controlled by means of external parameters. An example is the interdot coupling that can be tuned by external parameters far out of the regimes known for natural molecules. The ground-state interatomic distance is dictated, in natural molecules, by the nature of bonding [2] while such a restriction does not exist in artificial molecules. Most of the work has focused on the situation where the coupled QDs are in the tunneling regime so that the physics is dominated by Coulomb blockade effects [3, 4]. It was observed a pronounced anticrossing resonance scenario (called also avoided level crossing scenario) instead of a simple crossing one. Recently Rushforth *et al.* [5] studied the movement of electrons between the dots. Application of a voltage onto the gate between the dots allows to vary the length as well as the width of the wire connecting the dots. The study revealed evidence that electrons move between the dots via excited states of either the single dots or the double dot molecule.

In the present paper, we consider the ballistic transport through a double QD in the regime where Coulomb blockade effects can be neglected and where the transmission is resonant. The two single QDs are connected by a wire of finite length. This gives the possibility to vary the length or the width of the wire and to study the transmission through the double QD as a function of the wire's size and energy. When the length L of the wire is much larger than its width then the wire has at least one eigenmode with the energy $\epsilon \propto L^{-2}$. This mode appears additionally to the eigenstates $\varepsilon \propto R^{-2}$ of the two single QDs (where R is the radius of the dot) which may be equal to one another or different from one another. Such a double QD system allows therefore to investigate, among others, the quantum mechanical problem of the coupling of two identical quantum systems that is provided by a third quantum mechanical subsystem with an own energy spectrum. This system is the analogue of a molecule with hydrogen bonds.

Some years ago, the phase of the transmission amplitude has been measured in a double-slit interference experiment [6]. The results showed phase jumps by π between resonances which raised intensive theoretical work for an explanation [7, 8, 9, 10, 11, 12]. Most of these calculations associate the sharp phase drops with the occurrence of transmission zeros and relate them to the interference zeros of Fano resonances. In [12], it was shown however that the existence of a transmission zero is, indeed, a necessary condition for the phase jump but not a sufficient one. The sharp phase change bases, according to [12], on the destructive interference between neighboring resonance states and thus differs from the mechanism based on the Fano interference picture. Destructive interferences between neighbored resonances are considered also in [9, 11].

The Fano resonance phenomenon characterizes the interference between a single resonance with a relatively smooth background [13]. The interference processes in the regime of overlapping resonances are, however, much more complicated than those in the regime of isolated resonances. This has been demonstrated, e.g., in an experimental study of the conductance through a quantum dot in an Aharonov-Bohm interferometer [14] and in a theoretical study [15]. These results are another hint to the conclusion, drawn in [12], that the sharp phase changes observed in [6] are the result of processes being different from the simple Fano interference picture.

Here, we study the transmission properties of the double QD system when one lead is attached to the first single QD, another one to the second single QD, and both single QDs are connected by a wire of finite length L. Also in this system, transmission zeros appear. The special situation of a double QD is such that the transmission zeros of the whole system are determined by the zeros in the transmission through the single QDs. Since phase jumps in the transmission amplitudes are related to the transmission zeros, the mechanism of their appearance in a double QD system is expected to be different from that based on the simple picture of Fano resonances.

We will show in the present paper that transmission zeros of first order of a single 2d QD cause phase jumps by π in the amplitude of the transmission through this single QD. It depends on the spectral properties of both single QDs and on the manner they are connected to the wire and to the leads, whether or not the transmission zeros of the single QDs cause phase jumps of the transmission amplitudes of the double QD system. When the single QDs remain true 2d-systems in the double QD (as shown in Fig. 4) and have different energy

spectra, each transmission zero of each single QD causes a transmission zero of the same type in the double QD system. When the spectra of both single QDs are however equal (and their connection to the wire and the leads is the same as above), the corresponding transmission zeros of the double QD system are of second order. They give rise to two phase jumps, each by π, that compensate each other. When a resonance state crosses this transmission zero at a certain length of the wire, its decay width vanishes and a phase jump appears now due to the extremely narrow resonance. The transmission zeros do not depend on the length of the wire when there is only one channel for the propagation of the mode in the wire and in the leads.

In Sect. II, we present some numerical results for the transmission through a double QD that consists of two single QDs connected by a wire. The main features of the transmission are represented as a function of the length L of the wire inside the double QD: the transmission zeros are independent of L while many transmission peaks show some periodicity as a function of L. In the following sections, we study the transmission through a double QD in detail by using a simple model with only a few levels in both single QDs and one level in the wire. The description is based on the S matrix theory for the transmission through quantum dots [16]. In Sect. III, the formalism is derived and some typical numerical results are given and discussed. The spectral properties of the double QD are characterized by the (complex) eigenvalues of the effective Hamiltonian that describes the double QD when opened by attaching the two leads to it. This effective Hamiltonian is non-Hermitian, and its eigenvalues provide both the positions in energy and the decay widths of the states. The appearance of transmission zeros is determined by the spectral properties of the two single QDs.

The relation between transmission zeros and phase jumps is discussed in Section IV. Most results are obtained for the case that the two single QDs keep their 2d structure when connected to the leads and to the wire. The results show very clearly that the mechanism differs from that based on the simple Fano interference picture: the spectral properties of the states of the double QD system depend strongly on the length of the wire, while the transmission zeros do not depend at all on the length. The transmission zeros are of first order when the energy spectra of the two single QDs are different from one another, and of second order when the spectra of the two single QDs are identical. With the last section, we conclude the present study by mentioning some results for more complicated double QD

systems. In particular we consider the case that the widths of the leads and of the wire are different from one another. When the wire's width exceeds the lead's one, a few channels can propagate through the wire and the transmission zeros depend on the wire's length.

II. SINGLE CHANNEL TRANSMISSION THROUGH DOUBLE DOTS

Let us consider first a double QD consisting of two identical single QDs, for example, two circular dots, that are connected by a wire of the length L. For simplicity we choose the width of the wire d equal to the width of the leads, see Fig. 1 (a). The theory of transmission through such a system is given by Klimenko and Onipko [17]. If the dots are identical, the probability of the transmission for the single-channel case is

$$T = \frac{T_1^2}{T_1^2 + 4(1 - T_1)\sin^2(\phi + kL)} \tag{1}$$

where $T_1 = |t_1|^2$, t_1 is the complex amplitude of the transmission through the single QD, $\phi = arg(t_1)$, and k is the wave number related to the energy of the single-channel transmission as

$$E = k^2 + \pi^2. \tag{2}$$

All values are dimensionless via the characteristic energy $\frac{\hbar^2}{2m^*d^2}$ and the width d of the wire and the leads. In the expression (1), evanescent modes are ignored whose wave vectors are imaginary. That means, (1) can be used for $kL \gg 1$. The results shown in Fig. 1 are obtained from numerical calculations with $k > 3$. Here, formula (1) is applicable already for $L > 1$. Similar results for a system of two single QDs with different shape were obtained numerically by Pichugin [18].

The transmission probability demonstrates a few interesting features that are shown in Fig. 1 (b) - (d). The first is some periodical dependence of the transmission peaks on the wire length and on the energy. This dependence can be seen immediately in formula (1), and we will not discuss it further. The second feature are the transmission zeros. They do not at all depend on the wire length, see Fig. 1 (d) where the transmission probability T is shown in logarithmic scale. Also this feature follows directly from (1): the zeros of the transmission probability T_1 through the single QD lead directly to zeros of the total transmission probability T. The third feature concerns the peaks of the transmission probability. Fig. 1 demonstrates crossings and anticrossings of resonant peaks as observed
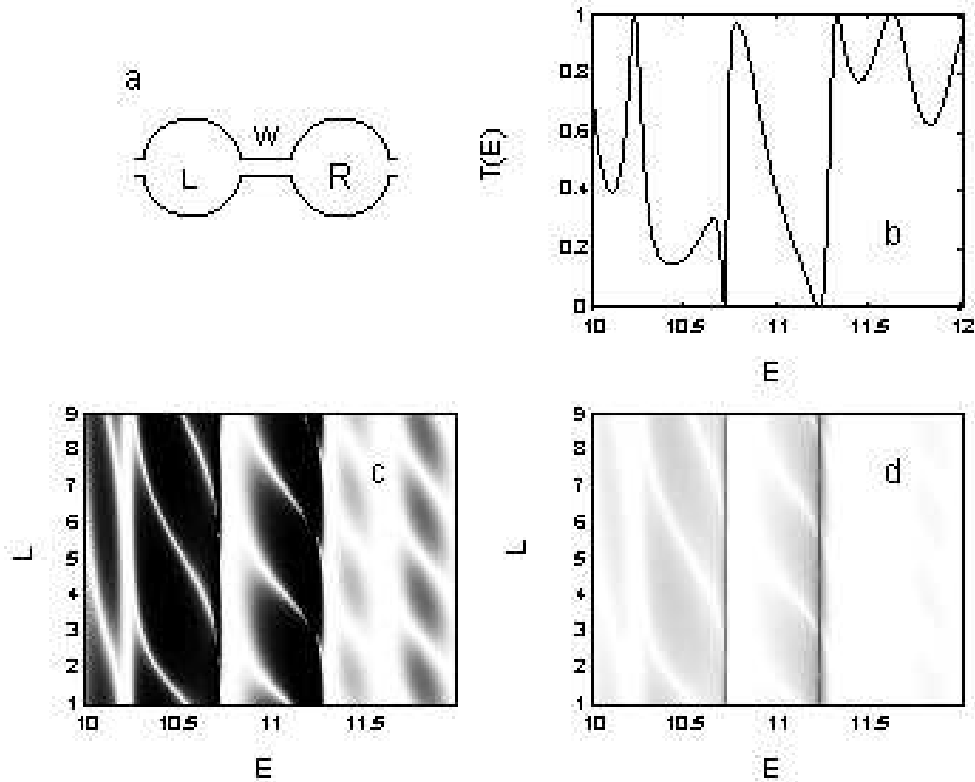
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FIG. 1: (a) The shape of the double QD that consists of two identical circular dots and a wire connecting the two dots. Numerical size of the double QD: radius $R = 40$ and width of the wire and leads $d = 8$. (b) The probability $T_1(E)$ for the transmission through one of the single circular dots versus energy. (c) The probability $T(E, L)$ for transmission through the double QD shown in (a) versus energy and length of the wire. (d) The same as (c) but $ln(T(E, L))$ in order to show clearly the zeros for the transmission through the double QD.

in experiments [3, 5]. Some of them are independent of the length L, as the transmission zeros, while other ones are dependent on L. The latter ones cross the L independent peaks as well as the zeros, but the behaviour in the vicinity of the crossing with a zero is different from that in the vicinity of the crossing with a maximum.

In the following, we will consider these features in detail. For this purpose, we use the periodicity (first feature) of the transmission picture that allows us to restrict the investigation to the transmission properties of a simple model with only a few states. The study is based on the S-matrix theory.

III. S-MATRIX DESCRIPTION OF THE TRANSMISSION THROUGH DOUBLE DOTS

A. Closed system consisting of two single dots connected by a wire

The Hamiltonian of the double QD shown in Fig. 1 (a) consists of three parts: two parts describe the two single QDs and a third one is related to the wire. The Hamiltonian of the two single QDs is formulated in standard way,

$$H_d = H_L + H_R = \sum_{n_L=1}^{N_L} \varepsilon_{n_L} |n_L\rangle\langle n_L| + \sum_{n_R=1}^{N_R} \varepsilon_{n_R} |n_R\rangle\langle n_R| , \tag{3}$$

where the indices L, R stand, respectively, for the left and right single QD with the energies $\varepsilon_{n_L}, \varepsilon_{n_R}$ and the Hilbert dimensions N_L, N_R. The wire is the third independent quantum mechanical subsystem described by the Hamiltonian

$$H_w = \sum_{n_w=1}^{N_w} \epsilon_{n_w}(L) |n_w\rangle\langle n_w| . \tag{4}$$

We assume that the eigenenergies $\epsilon_{n_w}(L)$ of the wire depend only on its length L. This offers the possibility for the energies of the wire to cross the eigenenergies of the single QDs. We assume further that the wire is coupled to, respectively, the left and right single QD via the matrices U_L, U_R of rank $N_L \times N_w$, $N_R \times d_w$. Then the total Hamiltonian has the following matrix form

$$H_B = \begin{pmatrix} H_L & U_L & 0 \\ U_L^+ & H_w & U_R^+ \\ 0 & U_R & H_R \end{pmatrix}. \tag{5}$$

The Hamiltonian (5) differs from those used in the literature [10, 11, 19] for the description of a double QD of similar shape by taking explicitly into account the third part (4) for the wire.

For the simplest case $N_L = N_w = N_R = 1$ and equal single QDs, the total Hamiltonian takes the following form

$$H_B = \begin{pmatrix} \varepsilon_1 & u & 0 \\ u & \epsilon(L) & u \\ 0 & u & \varepsilon_1 \end{pmatrix}. \tag{6}$$

The eigenvalues of this Hamiltonian are

$$E_{1,3} = \frac{\varepsilon_1 + \epsilon(L)}{2} \mp \eta, \quad E_2 = \varepsilon_1, \tag{7}$$

$$\eta^2 = \Delta\varepsilon^2 + 2u^2, \quad \Delta\varepsilon = \frac{\varepsilon_1 - \epsilon(L)}{2} \tag{8}$$

and the eigenstates read

$$|1\rangle = \frac{1}{\sqrt{2\eta(\eta + \Delta\varepsilon)}} \begin{pmatrix} -u \\ \eta + \Delta\varepsilon \\ -u \end{pmatrix}, |2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, |3\rangle = \frac{1}{\sqrt{2\eta(\eta - \Delta\varepsilon)}} \begin{pmatrix} u \\ \eta - \Delta\varepsilon \\ u \end{pmatrix}. \tag{9}$$

It is remarkable that one of the eigenenergies of the total system coincides with the energy ε_1 of the single QD. This fact remains also in the more general cases with higher dimensions.

Let us consider the case of two identical single QDs with the number N of states that are coupled via the wire. Then it follows $U_L = U_R$, if the wire is a straight one. The determinant which defines the eigenvalues of the total Hamiltonian is of rank $2N + N_w$,

$$\begin{vmatrix} E_1 - E & 0 & \cdots & U_{11} & U_{12} & \cdots & 0 & 0 \\ 0 & E_2 - E & \cdots & U_{21} & U_{22} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ U_{11} & U_{21} & \cdots & \epsilon_1(L) - E & 0 & \cdots & U_{12} & U_{11} \\ U_{12} & U_{22} & \cdots & 0 & \epsilon_2(L) - E & \cdots & U_{12} & U_{11} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & U_{21} & U_{22} & \cdots & E_2 - E & 0 \\ 0 & 0 & \cdots & U_{11} & U_{12} & \cdots & 0 & E_1 - E \end{vmatrix} = 0. \tag{10}$$

When $E = E_n$, $n = 1, \ldots, d$, two lines in (10) coincide. Therefore, among the $2N + N_w$ eigenenergies of the Hamiltonian (5), there are N eigenvalues which are equal to the eigenenergies of the single dots. Numerical examples for the eigenvalues of H_B with $N = 1$ and 2 are given by the solid lines in Fig. 3.

B.   S-matrix for the transmission through double dots: single QDs with one state.

The knowledge of the eigenstates of the closed quantum system allows us to formulate the S-matrix and the effective Hamiltonian in the manner described in [16]. Let us consider
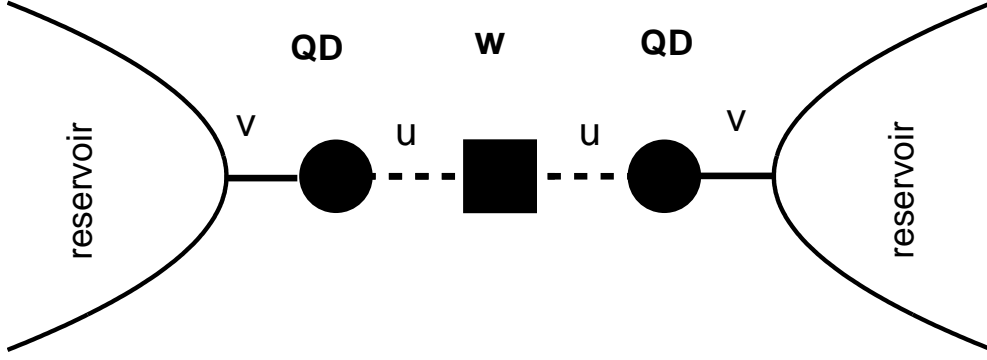
FIG. 2: Two single state QDs are connected to the wire w with the coupling constants u and to the reservoirs with the coupling constants v.

first the most simple case of the Hamiltonian (6). For the transmission through this system we imply two leads coupled to the reservoirs with the strength v, as shown in Fig. 2.

The coupling matrix has the following general form [16, 20]

$$V = \sum_m \sum_{C=L,R} \int dE \, V_m(E,C)|E,C\rangle\langle m| + H.C. \tag{11}$$

where $|m\rangle$ are the eigenstates of the closed system given in the present case by (9), and C enumerates the reservoirs with the states $|E,C\rangle$ normalized by

$$\langle E,C|E',C'\rangle = \delta(E-E')\delta_{C,C'}.$$

Obviously,

$$V_m(E,C) = \langle E,C|V|m\rangle = \sum_j \int_C dx \, \psi_C(x)\psi_m(j)\,\langle x|V|j\rangle \tag{12}$$

where j runs over the double dot system, x spans over the C-th reservoir, $\psi_C(x)$ are the eigenfunctions of the reservoirs, and $\psi_m(j)$ are the eigenfunctions of the closed double QD system. In our model we choose the couplings, that are shown in Fig. 2 by solid lines, to be fixed at some points: at $j = 1$, 3 of the left and the right single QD and at some points x_C which belong to the reservoirs. Moreover, we describe for simplicity the reservoirs as semi infinite one-dimensional wires in tight-binding approach [16]. As in [16], we take the connection points of the coupling to the reservoirs at the edges of the one-dimensional leads. Then the matrix elements (12) take the following form

$$V_m(E,L) = v\psi_{E,L}(x_L)\psi_m(j=1) = v\sqrt{\frac{\sin k}{2\pi}}\psi_m(1),$$

$$V_m(E, R) = v\psi_{E,L}(x_R)\psi_m(j = 3) = v\sqrt{\frac{\sin k}{2\pi}}\psi_m(3), \tag{13}$$

where k is the wave vector related to energy by $E = -2\cos k + 2$. For continual case the last equality is simply $E \approx k^2$. The effective Hamiltonian can be written as [16, 20]

$$H_{\text{eff}} = H_B + \sum_{C=L,R} V_{BC}\frac{1}{E^+ - H_C}V_{CB}, \tag{14}$$

where H_C is the Hamiltonian of the reservoir C and $E^+ = E + i0$. Substituting (13) into (14) we obtain for the matrix elements of the effective Hamiltonian

$$\begin{aligned}
\langle m|H_{\text{eff}}|n\rangle &= E_m\delta_{mn} + \sum_{C=L,R}\frac{1}{2\pi}\int_0^4 dE'\frac{V_m(E',C)V_n(E',C)}{E + i0 - E'} \\
&= E_m\delta_{mn} - v^2(\psi_m(1)\psi_n(1) + \psi_m(3)\psi_n(3))e^{ik},
\end{aligned} \tag{15}$$

where the states $\psi_n(j)$ are given in (9) and the indices $j = 1, 3$ mean, respectively, the left single QD ($j = 1$) and the right single QD ($j = 3$). Substituting (9) into (15) we obtain

$$H_{\text{eff}} = \begin{pmatrix} E_1 - \frac{v^2u^2e^{ik}}{\eta(\eta+\Delta\varepsilon)} & 0 & \frac{v^2ue^{ik}}{\sqrt{2}\eta} \\ 0 & \varepsilon_1 - v^2e^{ik} & 0 \\ \frac{v^2ue^{ik}}{\sqrt{2}\eta} & 0 & E_3 - \frac{v^2u^2e^{ik}}{\eta(\eta-\Delta\varepsilon)} \end{pmatrix}. \tag{16}$$

Next we calculate the (complex) eigenvalues of the effective Hamiltonian (16) that are related to the poles of the S matrix. The result is

$$\begin{aligned}
z_2 &= \varepsilon_1 - v^2e^{ik}, \\
z_{1,3} &= \frac{\varepsilon_1 + \epsilon(L) - v^2e^{ik}}{2} \mp \sqrt{\left(\frac{\epsilon(L) - \varepsilon_1 + v^2e^{ik}}{2}\right)^2 + 2u^2}.
\end{aligned} \tag{17}$$

For $u = 0$, the eigenvalues are $z_{1,3} = \varepsilon_1 - v^2e^{ik}$, $z_2 = \epsilon(L)$. The eigenvalue $z_2 = \epsilon(L)$ means that the wire has no other connection to the reservoirs as that via the single QDs.

In order to calculate the S-matrix we need the eigenstates of the effective Hamiltonian [16]

$$H_{\text{eff}}|\lambda) = z_\lambda|\lambda), \tag{18}$$

where $(\lambda| = |\lambda)^c$, $\lambda = 1, 2, 3$, c means transposition, and $(\lambda|\lambda') = \delta_{\lambda,\lambda'}$ is the biorthogonality relation for the eigenfunctions of the non-Hermitian Hamiltonian H_{eff} [21]. Then if follows from (16) (for $u \neq 0$):

$$|1) = \begin{pmatrix} a \\ 0 \\ b \end{pmatrix}, \quad |2) = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |3) = \begin{pmatrix} b \\ 0 \\ -a \end{pmatrix} \tag{19}$$

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with

$$a = -\frac{f}{\sqrt{2\xi(\xi + \omega)}}, \quad b = \sqrt{\frac{\xi + \omega}{2\xi}} \tag{20}$$

and

$$f = \frac{v^2 u e^{ik}}{\sqrt{2}\eta}, \quad \omega = -\eta + \frac{\Delta\varepsilon v^2 e^{ik}}{2\eta}, \quad \xi^2 = \omega^2 + f^2. \tag{21}$$

The knowledge of the eigenstates (19) of the effective Hamiltonian allows us to write the amplitude for the transmission through the double QD in simple form [16],

$$t = -2\pi i \sum_\lambda \frac{\langle L|V|\lambda\rangle(\lambda|V|R\rangle}{E - z_\lambda}. \tag{22}$$

The transmission probability is $T = |t|^2$. Substituting (13), (19) and correspondingly (9) into the matrix elements $\langle L|V|\lambda\rangle$ and $(\lambda|V|R\rangle$ we obtain

$$\langle L|V|2\rangle = \sum_m \langle E, L|V|m\rangle\langle m|2\rangle = \frac{v}{2}\sqrt{\frac{\sin k}{\pi}},$$

$$(2|V|R\rangle = \sum_m (2|m\rangle\langle m|V|E, L\rangle = -\frac{v}{2}\sqrt{\frac{\sin k}{\pi}},$$

$$\langle L|V|1\rangle = (1|V|R\rangle = v\sqrt{\frac{\sin k}{2\pi}}(\psi_1(1)a + \psi_3(1)b),$$

$$\langle L|V|3\rangle = (3|V|R\rangle = v\sqrt{\frac{\sin k}{2\pi}}(\psi_1(1)b - \psi_3(1)a), \tag{23}$$

where the eigenstates $\psi_m(j)$ are given in (9). Substituting finally (23) into (22) we obtain the transmission amplitude t.

The typical behavior of the transmission probability $T = |t(E, L)|^2$ versus energy E and length L is shown in Fig. 3. Here the energies ε_k of the two single QDs and the energy $\epsilon(L)$ of the wire are shown by dashed lines while the eigenenergies (7) of the double QD system are shown by solid lines. Since the eigenenergy E_2 of the double QD system coincides with the energy ε_1 of the single QDs, the last one is not shown in Fig. 3 (b). The eigenenergy of the wire is assumed to depend on the length L according to $\epsilon(L) = -1/2 - L/5$. This linear dependence is not decisive for the following discussion, see the Concluding Remarks.

We underline that the results presented in Fig. 3 follow from a simple model which describes the double QD system by two single-state dots connected by a wire. The wire is characterized by the only energy $\epsilon(L)$. When the coupling of the double QD system to the reservoir is relatively weak [meaning that the ratio v/u is small as in Fig. 3 (a,
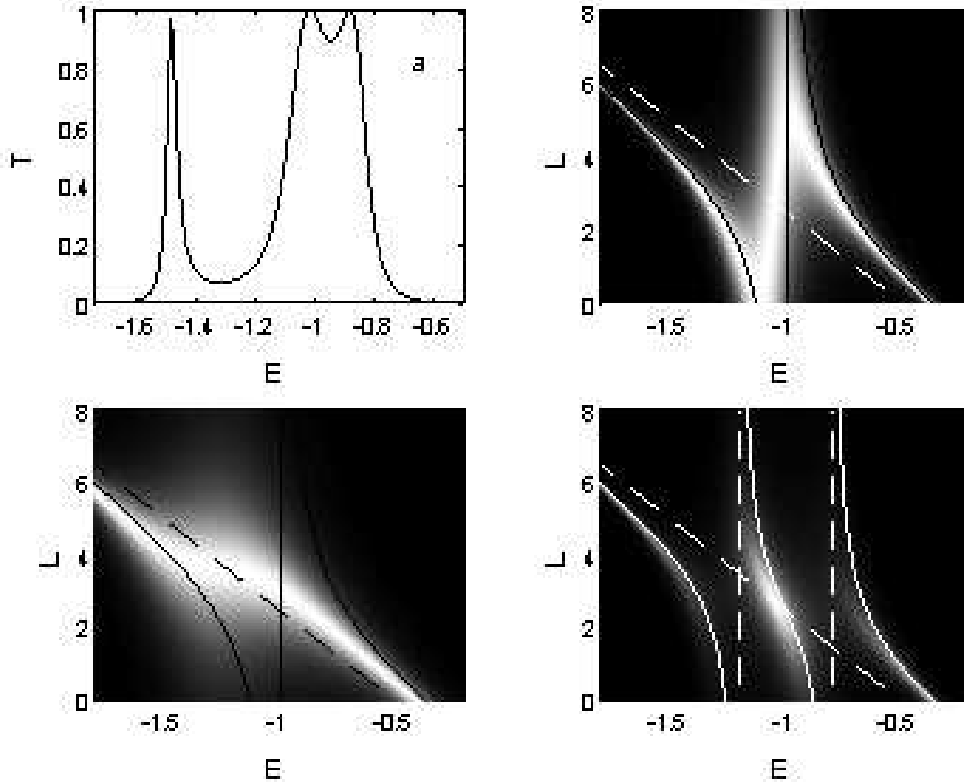
FIG. 3: The transmission probability T through the double QD shown in Fig. 2. (a) $\varepsilon_1 = -1$, $v = 0.3$, $u = 0.2$ and $L = 4$. (b) The same as (a) but the length L is not fixed. (c) The same as (b) but $\varepsilon_1 = -1$, $v = 0.6$, $u = 0.2$. (d) The same as (b) but $\varepsilon_1^L = -1.2$, $\varepsilon_1^R = -0.8$, $v = 0.3$, $u = 0.2$. The eigenenergies $E_k(L)$, $k = 1, 2, 3$, of H_B are shown by full lines while the energies ε_1 and $\epsilon(L) = -1/2 - L/5$ are given by dashed lines.

b, d)], the transmission probability follows the eigenenergies of the closed double QD, and we have resonant transmission. We can now compare Fig. 3 (b) with Fig. 1, and we see that the simple model, basic of Fig. 3 (a), is able to explain the peaks of the transmission probability. That means, the main features of the transmission picture in Fig. 1, are related to the crossing of the levels of the single QD with the energy level of the wire. As shown in Fig. 3 (b), (c) and (d) different scenarios of the resonant transmission peaks can be realized from the crossing to the anticrossing behavior in dependence on the parameters, basically on the coupling strength between the system and the attached leads and on the coupling strength between the dots and the wire.

We can further learn from Fig. 3 that the transmission through a system consisting of two dots that are connected by a wire, is characterized by the ratio v/u. Here, v is the

coupling strength of each single QD to the corresponding lead and u is the internal bonding of the two single QDs. Thus, v/u is the ratio between external and internal coupling of the states of the double QD via, respectively, the reservoir and the wire. In Fig. 3 (c), the coupling v between the double QD and the reservoirs exceeds essentially the coupling u of the two single QDs to the wire. In this case, the transmission is mainly given by the resonant transmission through the wire, and the two single QDs become parts of the reservoirs as it is directly seen from (17).

Moreover, Fig. 3 (d) shows the transmission through a double QD system consisting of two different single QD connected by a wire for the small ratio v/u. Also in this case, the transmission probability completely follows the eigenenergies of the double QD.

All the results obtained for a double QD with one-site single QDs do not show any transmission zeros in energy. In order to demonstrate the absence of zeros, we plotted in Fig. 3 (a) the energy dependence of the transmission probability for an arbitrary but fixed length L of the wire. The model underlying the results of Fig. 3 can be considered as a one-dimensional chain of three sites. It is in complete agreement with the consideration by Lee [8] that odd and even resonance levels alternate in energy in realistic 1d systems so that zeros in the transmission probability can not appear. The results of Fig. 3 correlate also with the consideration of a simple two site system [10, 16]. It has been shown for these systems that an architecture of the couplings between system and reservoirs, which violates the true one dimensionality of the closed system, gives rise to a zero in the transmission probability at a certain energy.

C. S-matrix for the transmission through double dots: single QDs with many states.

Here, we consider the transmission through a double QD when each single QD of the system is presented by two states as shown in Fig. 4. The Hamiltonian (5) of the closed
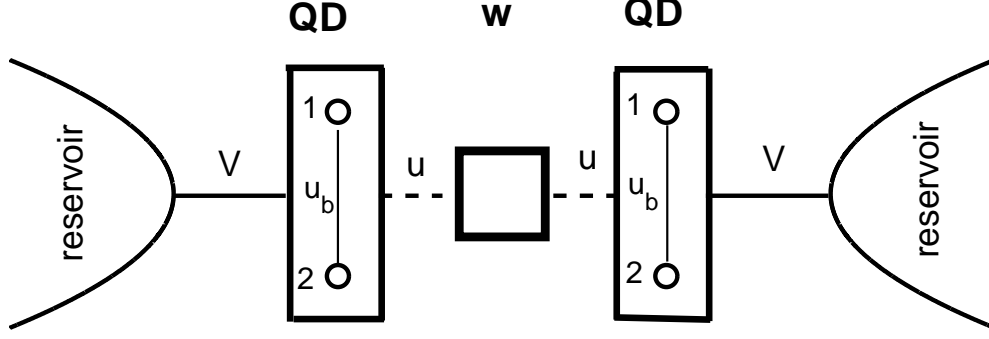
FIG. 4: The double dot system is connected to the reservoirs by the coupling constants v. The single dots are coupled to the wire by the coupling constants u.

double QD consisting of the two single QD and the wire is

$$
H_B = \begin{pmatrix}
\varepsilon_1 & 0 & u & 0 & 0 \\
0 & \varepsilon_2 & u & 0 & 0 \\
u & u & \epsilon(L) & u & u \\
0 & 0 & u & \varepsilon_2 & 0 \\
0 & 0 & u & 0 & \varepsilon_1
\end{pmatrix} . \tag{24}
$$

For simplicity we assume that all the coupling constants between the wire and the single QD are the same and are given by the constant value u.

The Hamiltonian (24) is written in the energy representation (3), (4). In order to specify the connection between the reservoirs and the single QDs, we have however to know the eigenstates of (24) also in the site representation. The Hamiltonian of the single QD in the site representation is

$$
H_b = \begin{pmatrix}
\varepsilon_0 & u_b \\
u_b & \varepsilon_0
\end{pmatrix} . \tag{25}
$$

The hopping matrix elements u_b are shown in Fig. 4 by thin solid lines. The eigenfunctions and eigenvalues are the following

$$
\langle j|\varepsilon_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} , \quad \langle j|\varepsilon_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} ,
$$

$$
\varepsilon_{1,2} = \varepsilon_0 \mp u_b. \tag{26}
$$

We introduce the projection operators

$$
P_L = \sum_{b_L} |\varepsilon_{b_L}\rangle\langle\varepsilon_{b_L}| , \quad P_w = |1_w\rangle\langle 1_w| , \quad P_R = \sum_{b_R} |\varepsilon_{b_R}\rangle\langle\varepsilon_{b_R}| \tag{27}
$$

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where $b_L = 1, 2$, $b_R = 1, 2$, and $|1_w\rangle$ is the one-dimensional eigenstate of the wire. Let E_m and $|m\rangle$ with $m = 1, ..., 5$ denote the five eigenenergies and eigenstates of (24), $H_B|m\rangle = E_m|m\rangle$. The elements of the left coupling matrix are

$$\langle L, E|V|m\rangle = \langle L, E|V P_L|m\rangle = \sum_{b_L}\langle L, E|V|\varepsilon_{b_L}\rangle\langle\varepsilon_{b_L}|m\rangle$$
$$= \sum_{j_L=1,2}\sum_{b_L}\langle L, E|V|j_L\rangle\langle j_L|\varepsilon_{b_L}\rangle\langle\varepsilon_{b_L}|m\rangle. \qquad (28)$$

Similar expressions can be derived for the right coupling matrix. Here we used the assumption that the left reservoir is connected only to the left single QD and the right reservoir only to the right single QD. As previously, the reservoirs are assumed to be semi infinite one-dimensional wires. Next we have to specify which sites of the left (right) single QD are connected to the left (right) reservoir. There are two possibilities.

(i) Assume the left reservoir is connected only to the first site $j_L = 1$ of the left single QD. Then (28) becomes with account of (26)

$$\langle L, E|V|m\rangle = v\sqrt{\frac{\sin k}{2\pi}}\sum_{b_L}\langle\varepsilon_{b_L}|m\rangle. \qquad (29)$$

A corresponding expression can be written down for the right coupling matrix if the right reservoir is connected to the first site of the right single QD.

(ii) We can assume that the reservoirs are connected to both sites of the single QDs with the same coupling constant v. Then the elements of the coupling matrices (29) are the following

$$\langle L, E|V|m\rangle = v\sqrt{\frac{\sin k}{2\pi}}\langle\varepsilon_1|m\rangle \qquad (30)$$

provided that the energy level ε_1 is the lowest in energy, see (26).

The most important difference between the previous $d = 1$ case and the present $d = 2$ one for the single QD is that the system is now no longer necessarily one dimensional. Therefore, zeros in the transmission probability may appear.

As it was shown above, Eq. (10), two eigenvalues of the Hamiltonian H_B coincide with the energies ε_1 and ε_2 of the single QD. The other three eigenvalues of (24) can be found by solving of a cubic equation. Also the finding of the eigenstates of (24) is a formidable task. In what follows, we consider therefore the transmission through a system with two states of each single QD numerically.
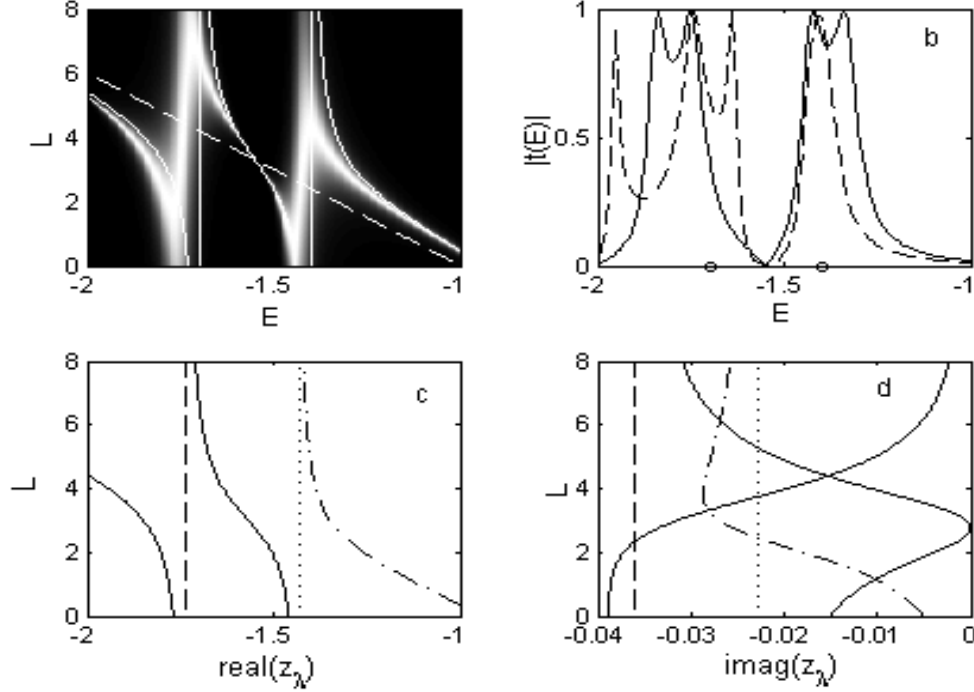
FIG. 5: (a) The transmission through a double QD with two identical single QDs that are connected by a wire according to Fig. 4. The eigenvalues of H_B are shown by full lines. $\varepsilon_1 = -1.7$, $\varepsilon_2 = -1.4$ and $\epsilon(L) = -1 - L/5$ (dashed line), $v = 0.3$, $u = 0.1$. (b) The modules of the transmission amplitude $|t(E, L)|$ for the same double QD as in (a) for fixed lengths $L = 2.75$ (solid line) and $L = 4$ (dashed line). The energies of the two single QDs are shown by circles. The real part (c) and imaginary part (d) of the 5 eigenvalues z_k of the effective Hamiltonian as a function of L for $E = -1.5$. Thin solid line: z_1, dashed line: z_2, thick solid line: z_3, dotted line: z_4, and dash-dotted line: z_5. At $L = 2.75$ the imaginary part of the third eigenvalue is equal to zero at all energies E.

In Fig. 5, the transmission probability versus energy E and length L of a double QD is shown for the case that both sites of the single QD are connected to the reservoir with the coupling matrix elements (30). The figure shows a zero in the transmission probability, indeed, see Fig. 5 (b). According to Figs. 5 (c) and (d), the positions and decay widths of the eigenstates 2 and 4 of the effective Hamiltonian are independent of the length L of the wire while those of the other states depend on L. The state 3, lying in the middle of the spectrum, crosses the transmission zero at $L = 2.75$. Here, the decay width of this state approaches zero for all energies E. The transmission zeros will be discussed in detail in the next section. Here, we remark only that resonance states with vanishing decay width are

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considered also by other authors. In [10], they are called ghost Fano resonances that appear in a double quantum dot molecule attached to leads. In atomic physics, the phenomena related to resonance states with vanishing decay width are known as population trapping [22]. They result from the interplay of the direct coupling of the states and their coupling via the continuum under the influence of, e.g., a strong laser field.

IV. ZEROS IN SINGLE-CHANNEL TRANSMISSION

In Fig. 6 (a), the transmission through a double QD system with two identical single QDs is shown, while Fig. 6 (b), shows the transmission through one of these single QDs (the lower curves correspond to the modules of the transmission amplitude and the upper curves to their phases). In the double QD system, the two single QDs are connected to the leads and to the wire as shown in Fig. 4. Comparing the two figures, we see that the transmission zero of the double QD coincides with that of the single QD. This result is in agreement with formula (1) for the single-channel transmission through identical dots. However there is a remarkable difference between the zeros in both cases as will be explained in the following.

Single QD [Fig. 6 (b, d)]: The transmission zero of the single QD is due to the destructive interference of the two neighboring resonance states [8, 12, 16] and is located between the energies of the single QD. It is caused by the unitarity of the S matrix with account of the fact that the leads are attached to the single QDs which are constituents of the double dot system [21]. Around the energy E_0, the transmission amplitude vanishes, $t(E_0) = 0$. Here $\text{Re}(t(E)) \sim (E - E_0)^2$ while $\text{Im}(t(E)) \sim \frac{d(\text{Re}(t(E)))}{dE} \sim (E - E_0)$. It holds therefore for the modulus of the transmission amplitude $|t(E)| \sim |E - E_0|$ near E_0, see Fig. 6(b), and $\frac{dt(E)}{dE}|_{E_0} \neq 0$. Thus, the phase of the transmission amplitude $\arg(t(E))$ jumps by π at E_0 according to [12]. The geometrical origin of this phase jump can clearly be seen in Fig. 6(d). By pathing through the origin of the coordinates $\text{Re}(t) = 0$, $\text{Im}(t) = 0$, the value $\arg(t)$ is not defined unambiguously. The phase jumps by $\pm\pi$, and the sign of the phase jump is not observable. We can call such a zero a first order zero.

Double QD [Fig. 6 (a, c)]: The zeros in the transmission through the double QD with two identical single QDs are of another type. They are of second order since it is $|t(E)| \sim |t_1(E)|^2$ in the vicinity of the energy $E = E_0$. It follows therefore $t(E) \sim (E - E_0)^2$ near E_0, see Fig. 6 (a). The energy evolution of the real and imaginary parts of the transmission amplitude is
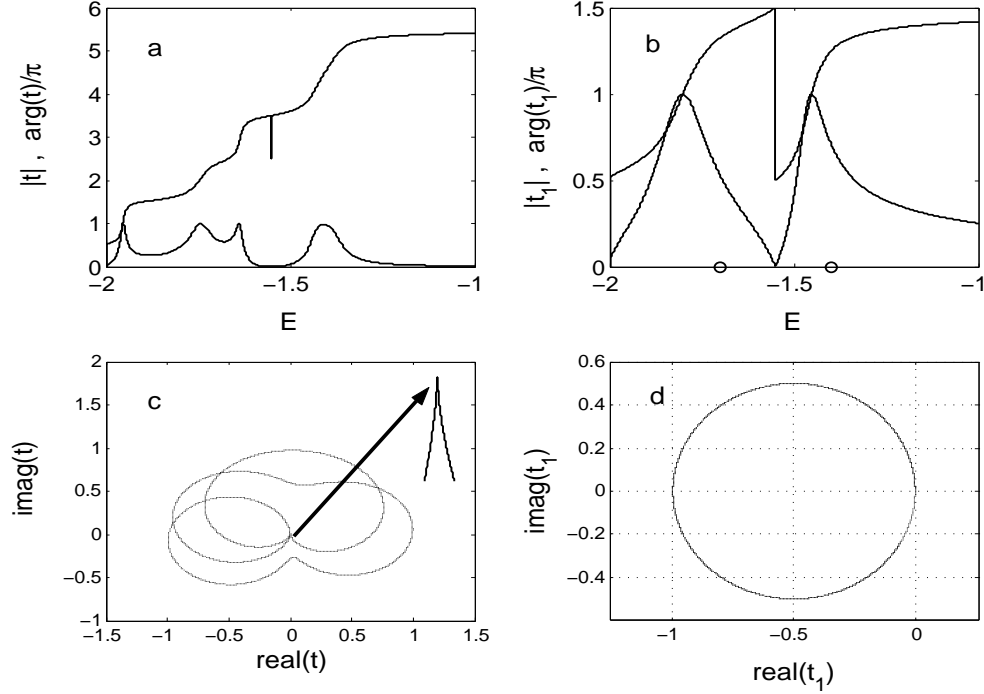
FIG. 6: (a) The modules $|t(E)|$ (lower curve) and the phase $arg(t)/\pi$ (upper curve) of the transmission amplitude for a double QD with two identical single QDs. The parameters are the same as in Fig. 5, and $L = 4$ as in Fig. 5 (b), dashed line. (b) The modules $|t_1(E)|$ (lower curve) and the phase $arg(t_1)/\pi$ (upper curve) of the transmission amplitude for one of the single QDs that is part of the double QD considered in (a). The energy positions of the single QD levels are shown by circles at the abscissa. (c) Evolution of imaginary and real parts of the transmission amplitude t of the double QD with energy. At the upper right corner, a zoomed fragment of the evolution is shown which demonstrates that the evolution has cusp-like behavior in the vicinity of the transmission zero. (d) The same as (c) but for the single QD. Here, the evolution is of standard type.

shown in Fig. 6(c). In the inset of the figure, the evolution of $\mathrm{Re}(t)$, $\mathrm{Im}(t)$ at the origin of the coordinate system is shown in zoomed resolution. It has a cusp-like behavior, and there is no phase jump at all. We present in Fig. 6 (a) the phase behavior of the transmission amplitude t that is a combination of two jumps with opposite sign, resulting in a zero phase jump at the point $E = E_0$. This result agrees with the general statement given by Barkay $et\ al$ [12], that phase jumps do not appear when $\frac{dt(E)}{dE}|_{E_0} = 0$ (as in our case) at the energy $E = E_0$.

According to formula (1), zeros of second order in the single-channel transmission of a double QD are given by zeros of first order in the transmission of the single QDs (that constitute the double QD) when they are identical. If both single QDs have N energy levels then $N - 1$ transmission zeros of second order will appear in the double QD system. A numerical computation for the particular case $N = 5$ confirms this conclusion (Fig. 7).
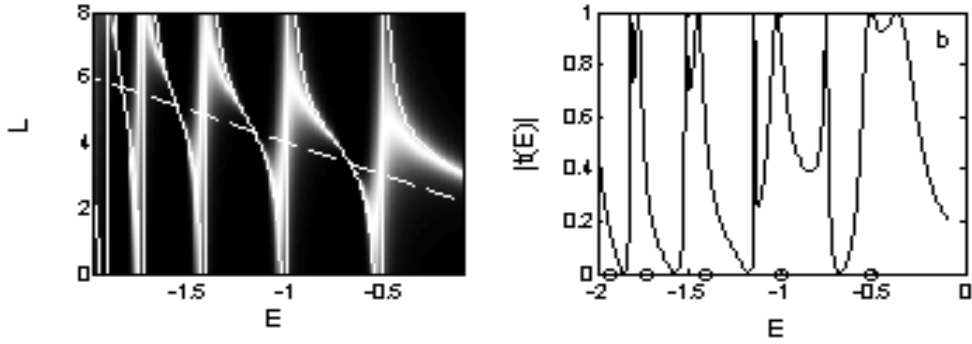

FIG. 7: (a) The transmission through a double QD consisting of two identical single QDs with $d = 5$ states that are connected by a wire, versus energy and length of the wire. The eigenvalues of H_B are shown by thin lines while the energy $\epsilon(L) = 1 - L/2$ of the mode in the wire is shown by the dashed line. $v = 0.5$, $u = 0.2$. (b) Energy dependence of the modules of the transmission amplitude for $L = 4$. The energy levels of the single QD are shown by circles at the energy axis, $\varepsilon_L = -2\cos(\pi n/6)$, $n = 1, 2, \ldots, 5$.

Next we will consider the transmission through a double QD consisting of two different single QDs coupled to the wire and to the leads as shown in Fig. 4. When each single QD has N states, the number of zeros in the transmission through the double QD is, according to (1), $2(N - 1)$. This conclusion is demonstrated by the results of numerical calculations shown in Fig. 8. Here, the two two-site single QDs are chosen to be different from one another what can be achieved by either different coupling constants u between the single QDs and the wire or by different energies of the levels of the two single QDs. We have chosen the latter possibility.

In Fig. 8, we see two transmission zeros of first order. The phase jump is $-\pi$ at the first zero and π at the second zero. Considering the transition $\varepsilon_k^l \to \varepsilon_k^r$ with $k = 1, 2$, we see that the transmission zeros will approach each other with the consequence that the transmission zero turns over into a second order zero. The phase jumps annihilate each other as shown in Fig. 6 (a).
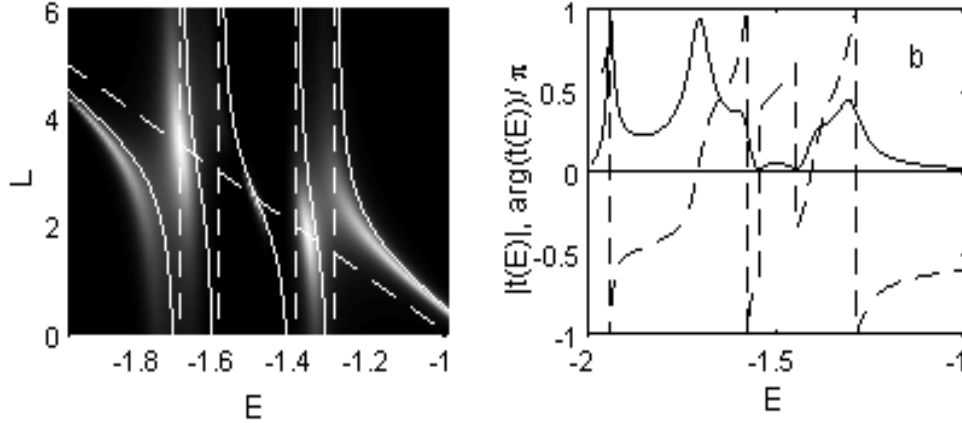
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FIG. 8: (a) The transmission through a double QD with different single QDs connected by a wire, and (b) the energy dependence of the modules (solid line) and of the phase $arg(t)/\pi$ (dashed line) of the transmission amplitude for this double QD system at a fixed length $L = 4$ of the wire. The energy levels of the left single QD are $\varepsilon_k^L = -1.7, -1.4$, while those of the right single QD are $\varepsilon_k^R = -1.6, -1.3..$ Further, $\epsilon(L) = -1 - L/5$, $v = 0.3$, $u = 0.1$. The full lines in (a) are the eigenvalues of H_B while the dashed lines are the energies ε_k^L, ε_k^R, and $\epsilon(E)$.

We consider now the evolution of the modules of the transmission amplitude and the corresponding phase shifts when the decay width of one of the states approaches zero. The results shown in Fig. 9 are performed for the double QD system the transmission of which is shown in Fig. 5 together with the eigenvalues z_k of the effective Hamiltonian H_{eff}, Eq. (14), as a function of L. The latter ones are related to the poles of the S-matrix. At $L = 2.75$, the third eigenstate crosses the energy of the transmission zero, and its decay width $\text{Im}(z_3)/2$ approaches zero. As long as $L \neq 2.75$ and $\text{Im}(z_3) \neq 0$, the phase of the transmission amplitude varies by π more or less smoothly, according to the phase shift caused by a resonance state with a finite decay width. When $L \to 2.75$ and $\text{Im}(z_3) \to 0$, the phase jumps by π due to the vanishing decay width of the resonance state. Therefore, we have also in this case a phase jump of the transmission amplitude by π. Correspondingly, the transmission zero becomes of first order at $L = 2.75$, see Fig. 5(b). That means the resonance state whose decay width vanishes when crossing the energy of the transmission zero, restores the first order of the transmission zero as well as the phase jump by π.

The connection of the two single QDs to the leads and to the wire may differ from that shown in Fig. 4. When one of the single QDs loses its 2d-character by the manner it is
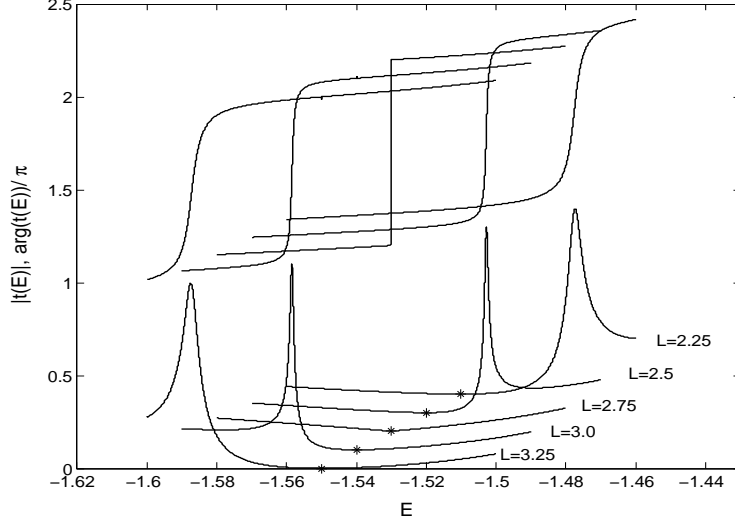
FIG. 9: The energy dependence of the modules $|t(E)|$ (bottom) and of the phase $arg(t(E))/\pi$ (top) of the transmission amplitude for $L = 2.25, \ 2.5, \ 2.75, \ 3.0, \ 3.25$. The other parameters are the same as those in Fig. 5. The transmission zeros are denoted by stars. They are of second order. The ordinate is shifted every time by 0.1 when L is changed by 0.25. All phases are shifted by π.

integrated in the double QD system, only transmission zeros of first order appear in the double QD. When both single QDs are included as 1d dots, the double QD system has no transmission zero at all. In this case, the whole system behaves as a 1d chain of sites without any transmission zeros.

V. CONCLUDING REMARKS

From the present study, we conclude that the simple model used by us for the description of a double QD system consisting of two single QDs coupled by a wire, is efficient and describes qualitatively the features of the resonant transmission through a realistic double QD of the same structure. The difference between the transmission through the realistic double QD shown in Fig. 1 and the model cases shown in Figs. 3, 5, 7 and 8 consists, above all, in the fact that all features of the simple model are multiply repeating in the realistic case. These multiple effects in realistic cases are related, obviously, to the large dimension of the single QDs and to the higher number of eigenmodes of the wire inside the double QD system.

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The advantage of the simple model described by S matrix theory is that it allows a clear discussion of the main features of the transmission, especially of the transmission zeros and of the phase jumps related to them. Of course, the model can give only qualitative results that do not agree quantitatively with the numerical results (Fig. 1) obtained for the realistic double QD system. However there is a large room to further develop the model. First, we can take the eigenenergies of the wire for the single channel propagation as

$$\epsilon_n(L) = \frac{\pi^2}{d^2} + \frac{\pi^2 n^2}{L^2}, n = 1, 2, \ldots \tag{31}$$

where d is the width of the wire. The first term in (31) is related to the first-channel propagation in the wire. Moreover we can take into account that the eigenstates of the wire have the form

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin(\pi n x / L). \tag{32}$$

Then u can be calculated in the same way as v [16, 20]

$$u_n(L) = u_0 L^{-1/2} \psi_n'(x) \mid_{x=0,L} = u_n L^{-3/2}, \tag{33}$$

and the Hamiltonian (4) reads

$$H_w = \epsilon_1(L)|1\rangle\langle 1| + \epsilon_2(L)|2\rangle\langle 2|. \tag{34}$$

In our calculations we have chosen the widths of the wire inside the double QD and the widths of leads attached to the QD to be the same. Thereby, the leads and the wire both support only single channel transmission through the double QD. Experimentally, however, the width of the wire varies, usually, by applying gate voltages [3] while the length of the leads remains fixed. In order to model this case, we can consider two energy levels of the wire one of which is related to the first channel propagation (31) and the other one to the second channel propagation

$$\epsilon_{n'}(L) = \frac{4\pi^2}{d^2} + \frac{\pi^2 n'^2}{L^2}, n' = 1, 2, \ldots. \tag{35}$$

When the wire's width d exceeds the lead's width, we can take one energy level (31) (say, $n = 2$) together with another one from (35) (say, $n' = 1$) in such a manner that they cross at a certain length L_0, $\epsilon_n(L_0) = \epsilon_n'(L_0)$.

The numerical results obtained for the transmission probability (Fig. 10) for such a case are the following. For single channel propagation in the wire, the transmission features including the transmission zeros are similar to those discussed above. The number

of transmission zeros remains unchanged, but the number of transmission peaks is doubled corresponding to the two modes in the wire. These results correspond to those obtained for the single channel transmission through a realistic double dot system (Fig. 1). The situation
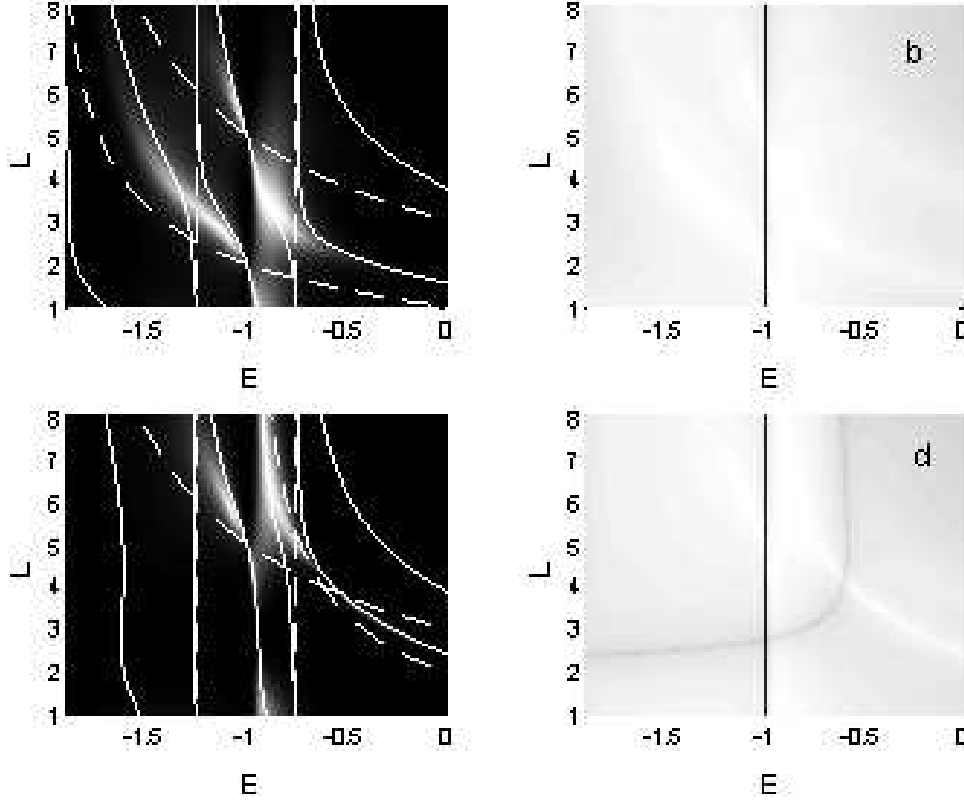

FIG. 10: The transmission probability (a,c) and its logarithm (b,d) for a double QD with a wire that has two energy levels. The single QDs have eigenenergies $\varepsilon_k = -1.25, -0.75$. The coupling strengths u between the single QDs and the wire are taken according to (33), $u = 0.2, v = 0.6$. In (a) and (b), the first-channel propagation is shown with the two energies of the wire given by (31), $n = 1, 2$. In (c) and (d), the two channel propagation in the wire is shown with the energies $\epsilon_1(L) = 4\pi^2/L^2$ and $\epsilon_2(L) = 1 + \pi^2/L^2$ that are crossing. The dashed lines show the eigenenergies of the isolated wire and the single QDs while the solid lines show the eigenenergies of the closed double QD system.

is however another one when the wire can support two channel propagation. In this case, the number of transmission zeros is doubled. One of the lines of the transmission zeros does not depend on the wire length L (as in the model calculations of Sect. IV), but the other one depends on L and crosses the first line of the transmission zeros. The multi channel

propagation induced by a variable width of the wire can lead, therefore, to an essentially more complicated picture of the transmission zeros. The picture of transmission zeros as a whole remains however comprehensible on the basis of the results obtained in the framework of the simple model considered above.

It is experimentally easier to vary the wire's width than its length. It is important therefore to mention that the width d and length L of the wire are equivalent for the energy levels of the multi-channel wire according to Eqs. (31) and (35). Therefore, the transmission probability versus energy and length shown in Fig. 10 can be qualitatively considered as the transmission probability versus energy and width of the wire.

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